MS19-1-3 Comparative study of in-house and synchrotron X-ray electron densities of molecular crystals #MS19-1-3

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Abstract
In this study, the data quality of a range of available in-house single crystal X-ray diffractometers was tested against synchrotron data on their ability to produce an accurate Multipolar Model (MM) of the electron density of the archetypical molecular crystal melamine. The instruments tested include the BL02B1 beamline at the SPring-8 synchrotron, state-of-the-art in-house diffractometers Rigaku Synergy-S, STOE Stadivari and the older Agilent Supernova. The specific details for obtained datasets can be seen in the table.

Overview of the six different datasets used for the MM comparison. At SPring8 data was collected at two different temperatures, and two different sources were tested at the Synergy-S.

	SPring8		Synergy-S		Stadivari	Supernova
Detector	Pilatus CdTe		HyPix arc100		Eiger CdTe	CCD
Wavelength [Å]	0.25		0.71 (Mo)	0.56 (Ag)	0.71 (Mo)	0.71 (Mo)
Temperature [K]	25	100	100	100	100	100

Preliminary analysis show that even though the data quality varies slightly between the six data sets, there is virtually no difference between the resulting multipole models. All datasets provide a reliable MM with great data quality (>20 (>7 for supernova) and redundancy >7), high resolution (>1.18 $Å^{-1}$), low R-factors (<3%) and low min/max residuals (<0.3 $e/Å^3$). Residual density map (ρ_{obs}-ρ_{calc}) and deformation density map (ρ_{MM}-ρ_{IAM}) for the six different datasets can be seen in the figure. Contour lines are shown at 0.1 $e/Å^3$. The residual density maps are shown at the highest common resolution cutoff of 1.18 $Å^{-1}$. Deformation density maps are calculated to the full resolution.The noise level is significantly higher for the Supernova with an old CCD detector as seen in the residual density map in the figure, but it has a random nature, suggesting low impact on the validity of the MM. The deformation density map in the figure obtained from the SPring8 100K dataset has some abnormal features in the upper part of the ring, suggesting minor systematic flaws. In the present case the SPring8 25K, Synergy Mo and Ag datasets seem to be of (slightly) higher quality among six quite excellent MMs.

Residual- and deformation density maps.